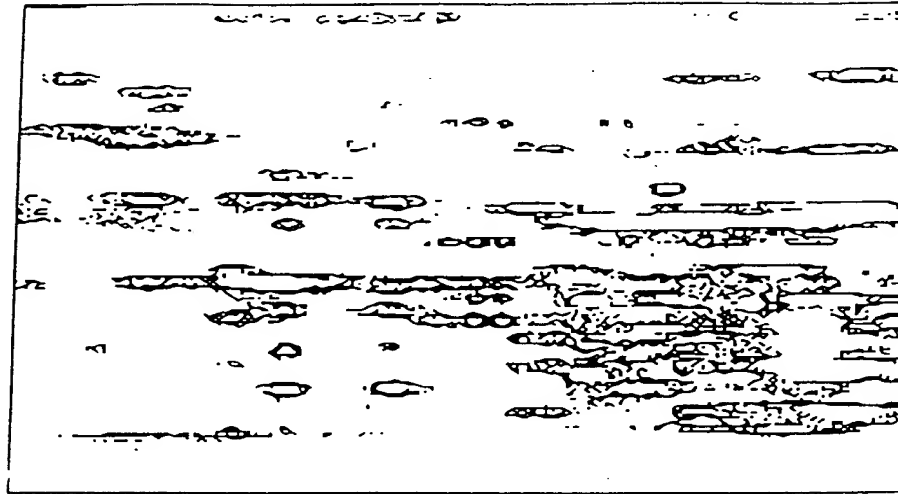


FIGURE 1A



05983020 102201

FIGURE 1B

FO220T" 020E8660

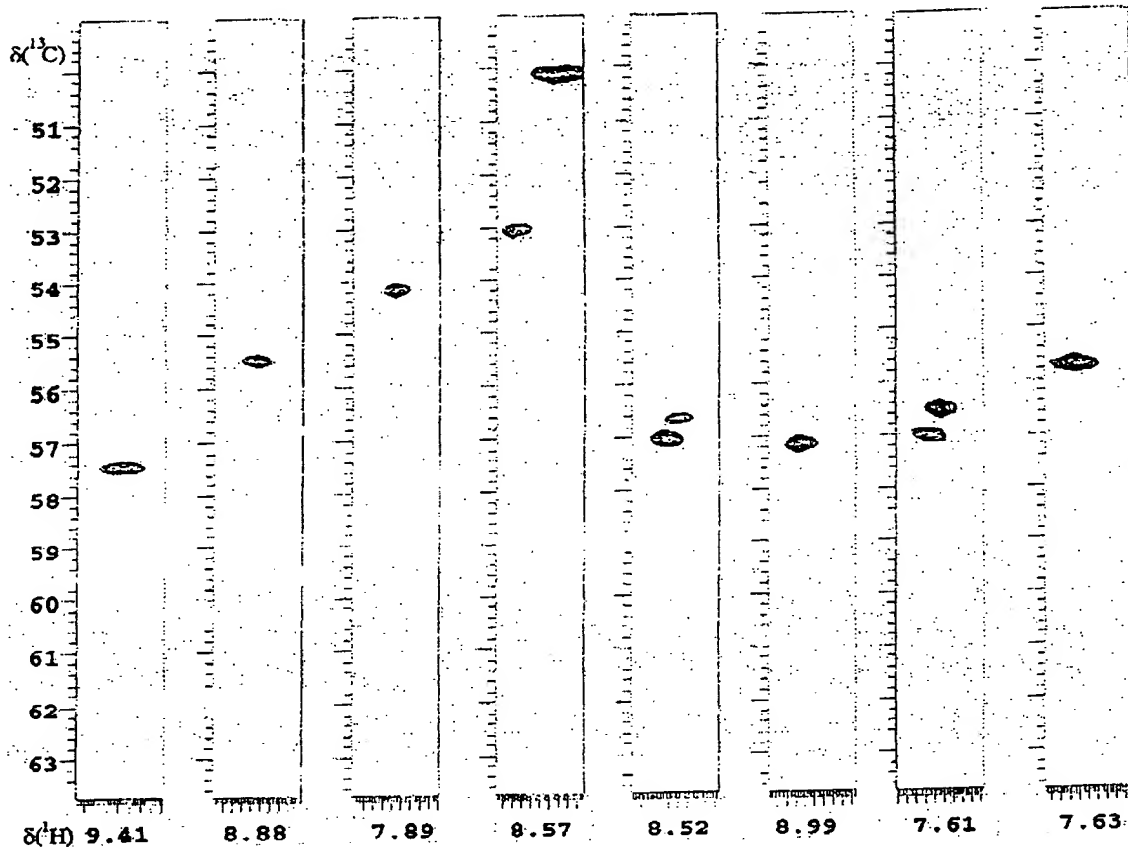
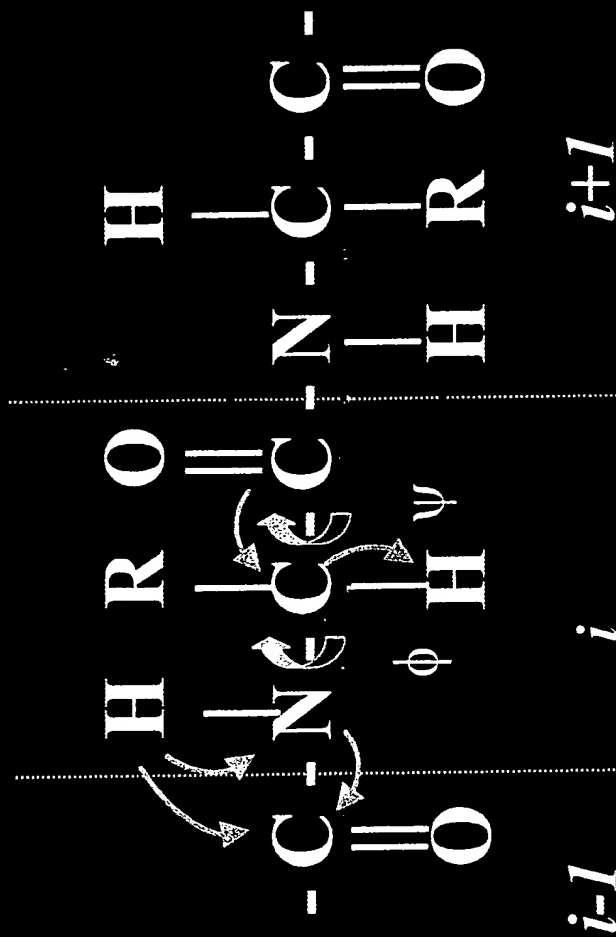


FIGURE 2

Dipolar Couplings That Depend Only on $\phi(i)$ and $\psi(i)$



Search ϕ and ψ Until Measured Couplings = Theoretical Couplings

FIGURE 3

Packing Secondary Structural Elements

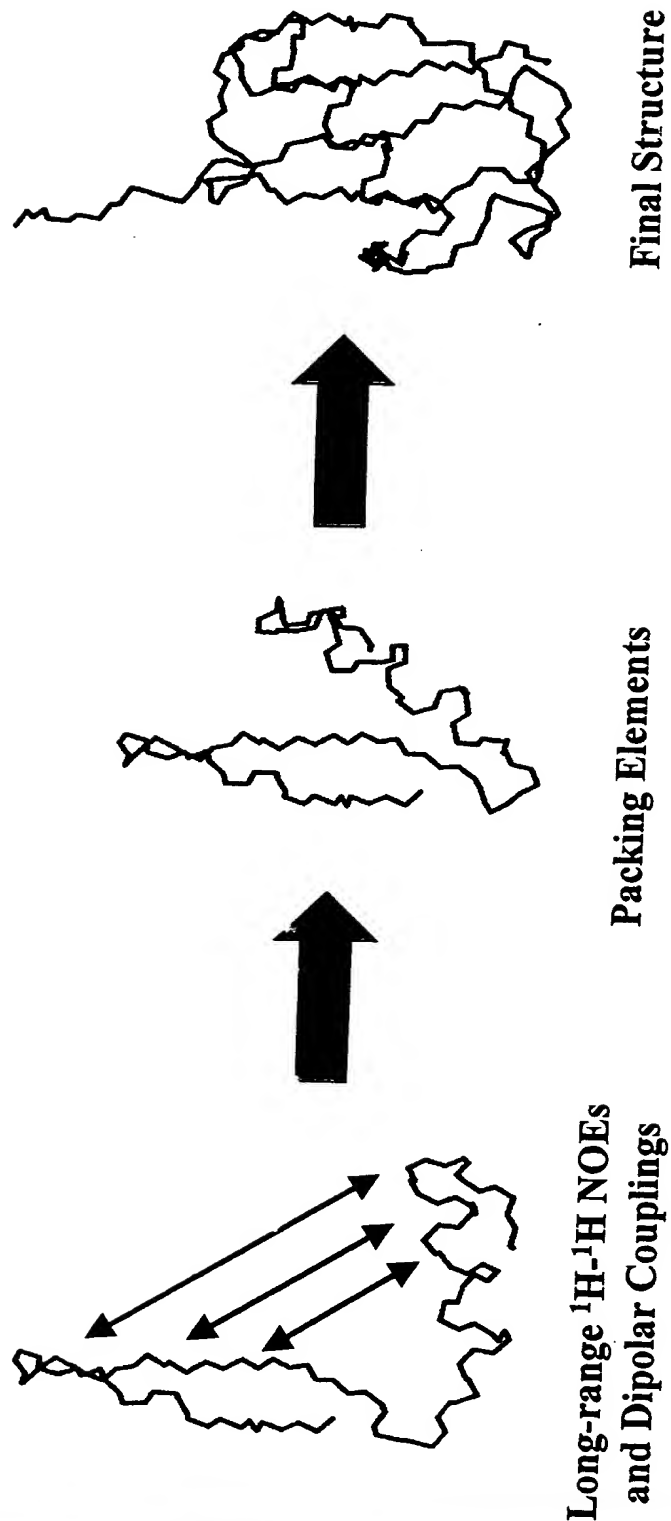
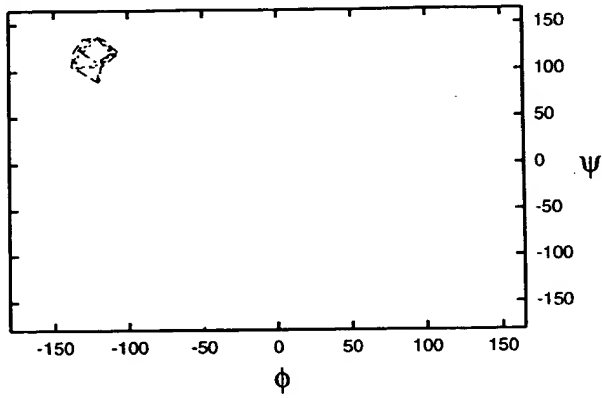


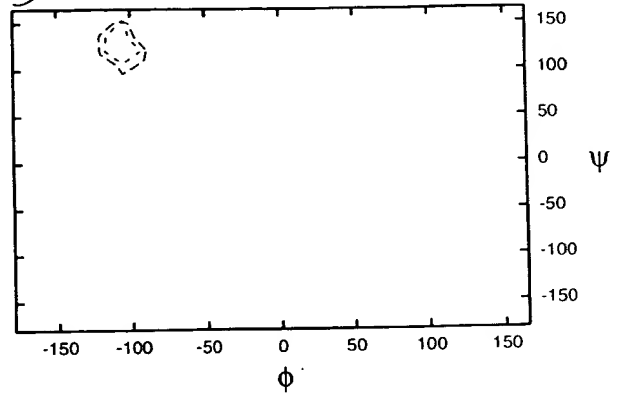
FIGURE 4

Examples of residues in β -sheet regions

A

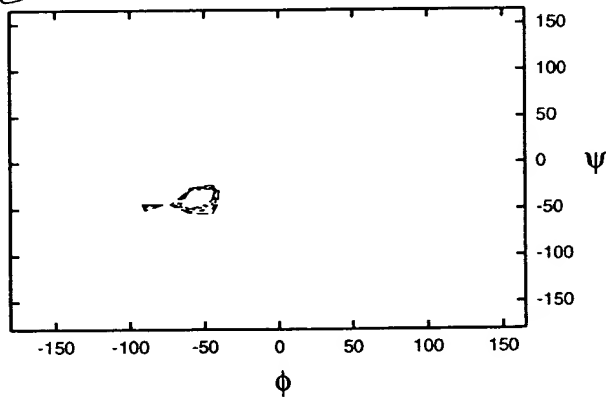


B

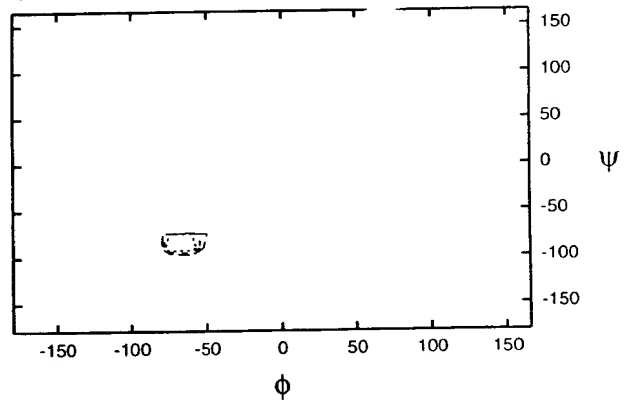


Examples of residues in α -helix regions

C

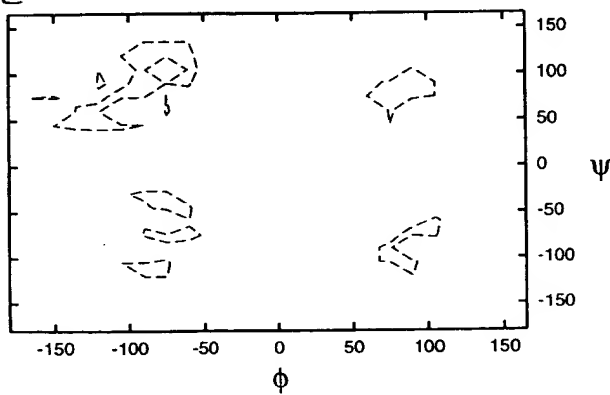


D



Example of residue in loop region

E



0998300-10201
T02207-020E8660

1022207-02088660

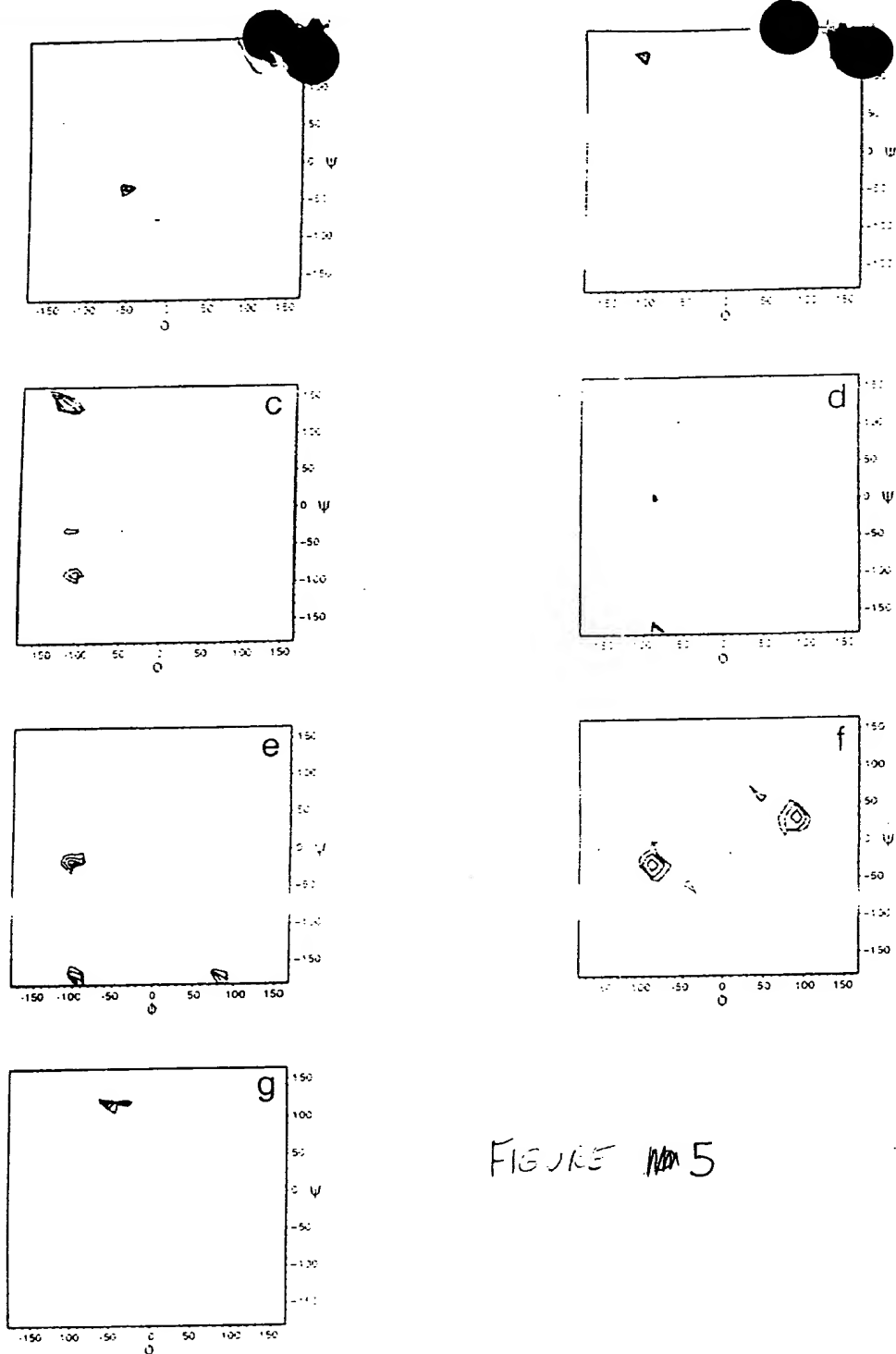


FIGURE 5

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RAPID DETERMINATION OF PROTEIN...
Atty. Dkt. No. 1496-205
Figure 5 of 13

09983020-102201

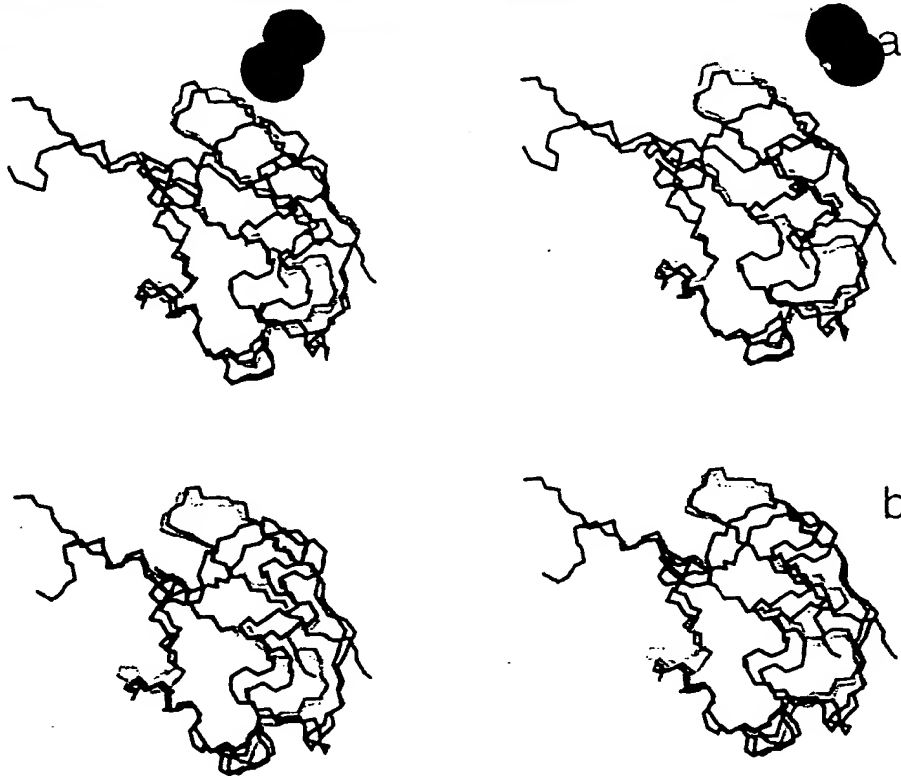


FIGURE 6

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RAPID DETERMINATION OF PROTEIN...
Atty. Dkt. No. 1496-205
Figure 6 of 13

Calculate ϕ, ψ angles
for each peptide pair
using experimental
residual dipolar couplings

Fold Linear sequence
with dihedral angle
and backbone NOE
restraints

Refine structure
using NOE and
dipolar coupling
restraints

[illegible]

Dipolar Couplings - Powerful Structural Constraints

H θ

B₀

C

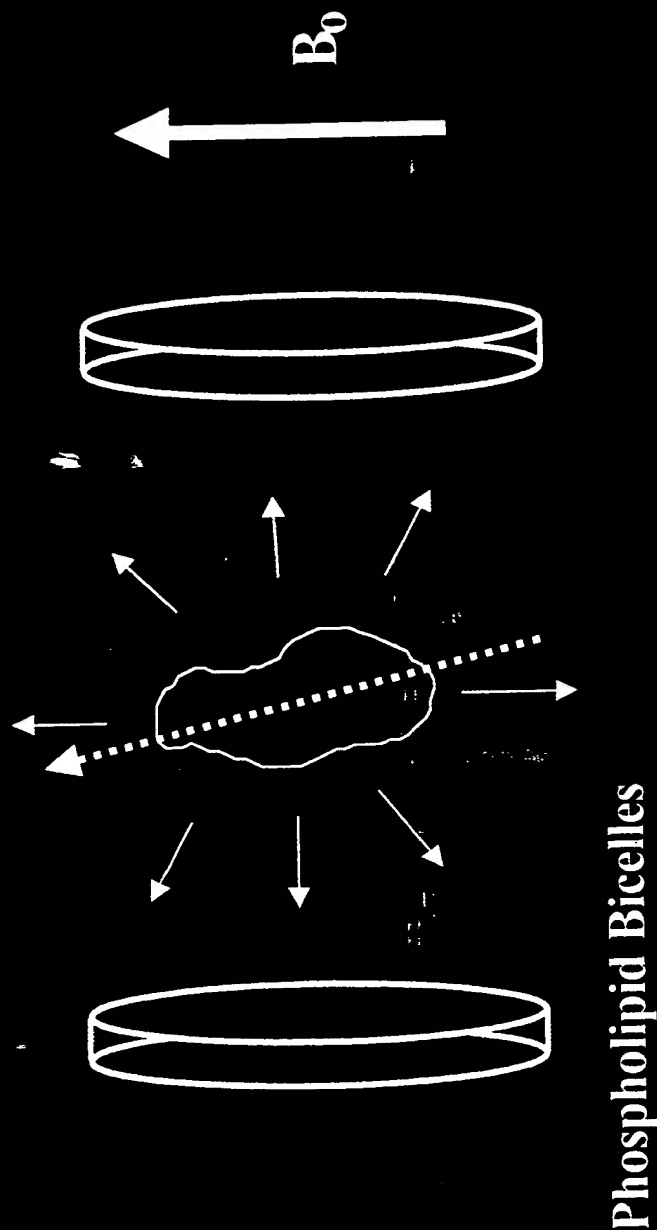
r

$$D \propto (3 \cos^2 \theta - 1) / r^3$$

J + D (Hz)



Measurement of Dipolar Couplings Requires a Weakly Aligned Molecule



J (Hz)

22° C: Isotropic (no alignment)

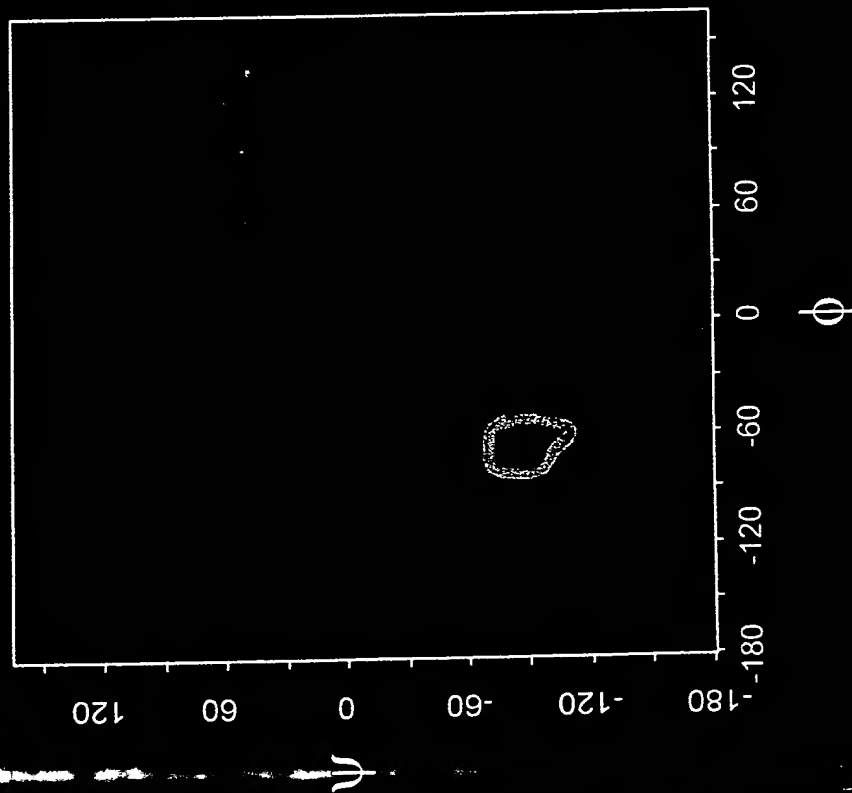
$J + D$ (Hz)

35° C: LC Phase (alignment)

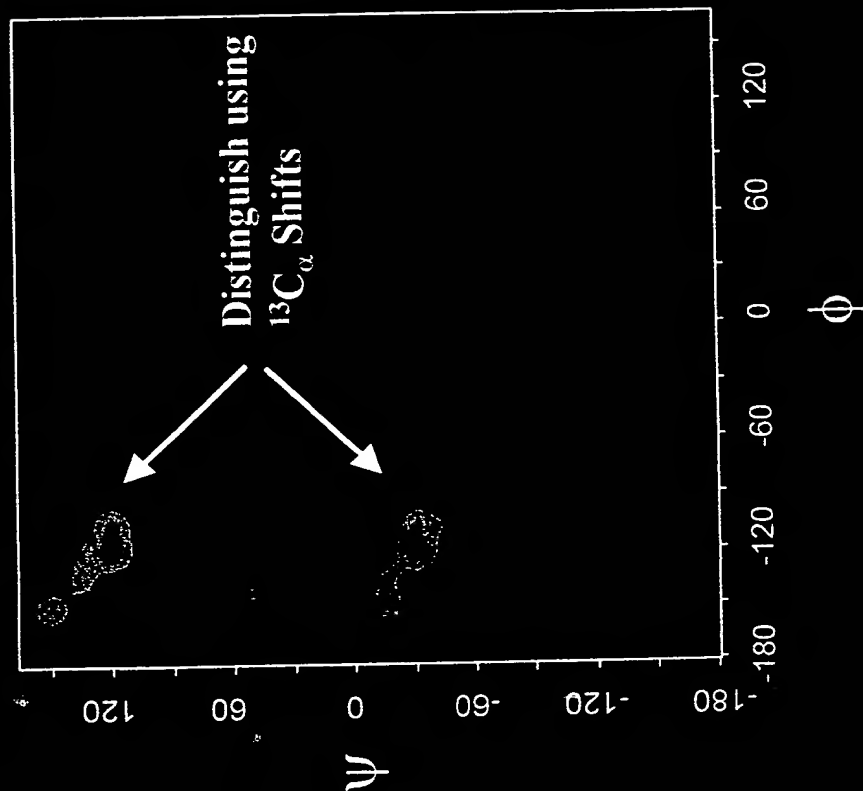
FIGURE 10

ϕ, ψ Mapping Using Residual Dipolar Couplings

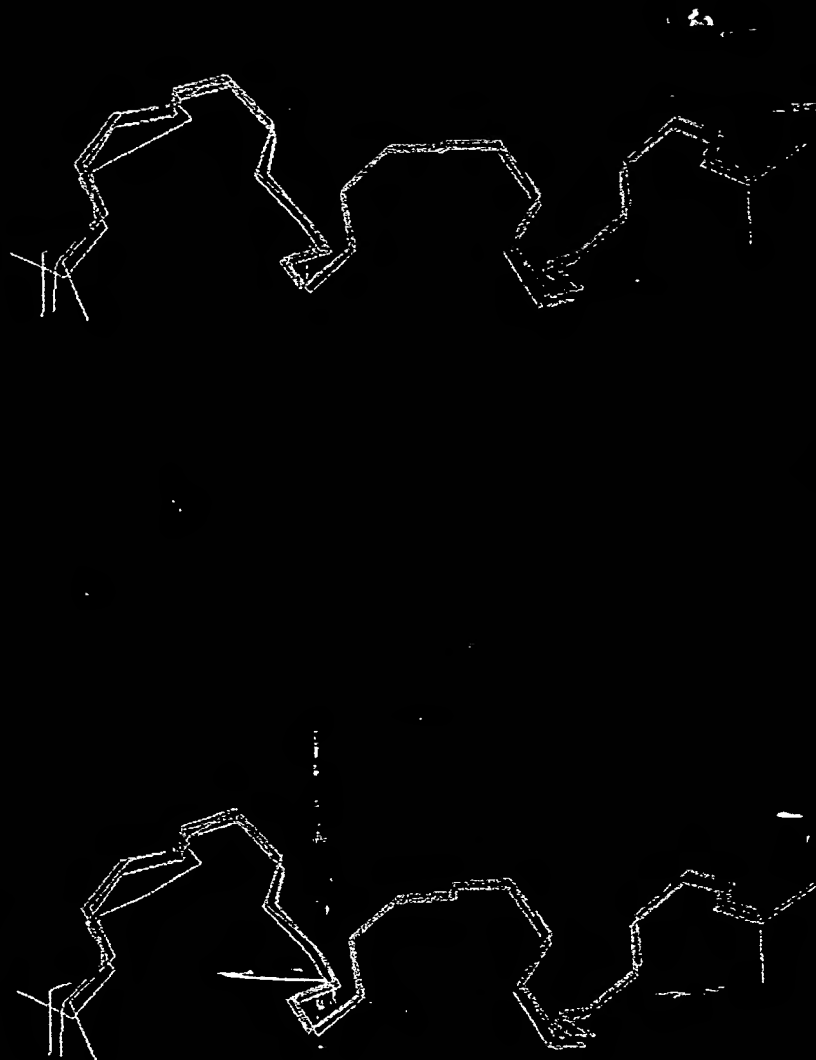
Val 26



Ile 33



NMR vs. Crystal Structure of α -helix (24-34) Ubiquitin



NMR — Crystal

FIGURE 11

NMR vs. Crystal Structure of β -sheet (3-15) Ubiquitin

FIGURE 12



NMR — Crystal

FIGURE 13

Crystal Structure vs. NMR Global Fold - Ubiquitin

